Power and group velocity

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Here we make use of the Hellmann-Feynman theorem, with the aim to calculate macroscopic quantum velocities instead of forces, and we show how it is possible to derive the expression of the work per unit time per unit volume (power density) done by a static external uniform electromagnetic field interacting with a quantal body.

INTRODUCTION

The problem of the *dielectric* and *magnetic* response of matter, in condensed matter physics, have been intensively studied in the last decades[1]-[12] (and references therein).

Here we show that making use of a reformulation of the Hellmann-Feynman theory, it is possible to derive several useful physical properties of a crystalline material in a direct and simple way. As a matter of example we shall show how to derive the expression of the group velocity of an electronic system interacting with an external uniform magnetostatic field, and how to obtain the expression of the electronic power density.

Let us start our discussion from a fundamental level by briefly reviewing the definition of *stationary state* or equivalently *steady state* of a quantal body (QB), as better stated in [13, 15, 18].

Let us consider the time-dependent Schrödinger equation

$$\begin{aligned} i\hbar\frac{\partial\Psi}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}}\Psi + V(\mathbf{r},t)\Psi \\ &= (T+V)\Psi = H_0\Psi \end{aligned} \tag{1}$$

where Ψ is the state of the system, T the kinetic energy operator and V the potential energy.

A considerable simplification of equation (1) is obtained if the potential energy is time independent, i.e $V(\mathbf{r},t) = V(\mathbf{r})$. In this case it is possible to express the general solution of eq.(1) as a sum of products of functions of $\mathbf{r}$ and t separately. Without entering into details, the time dependence of the wave function can be expressed as

$$\Psi(\mathbf{r},t) = u(\mathbf{r})e^{-i\frac{Et}{\hbar}} \tag{2}$$

being $u(\mathbf{r})$ the eigen function of the following differential equation [18]

$$-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}}\Psi + V(\mathbf{r})u(\mathbf{r}) = Eu(\mathbf{r}) \tag{3}$$

and E is the corresponding eigen value.

Eq.(3) formally defines a stationary state (see also [13, 15, 18]) for a system where the Hamiltonian assumes the form $H = T + V$. A more general definition of a steady state is

$$H\Psi = E\Psi \tag{4}$$

where H is the Hamiltonian of a quantal body, and H is either self-adjoint or hermitian (see [13, 15, 18]). In the following we shall frequently make use of the concept of steady states.

HELLMANN-FEYNMAN THEOREM

In 1939 R.P. Feynman[15] developed formulas to calculate forces in a quantum system, that nowadays take the name of Hellmann-Feynman theorem[15].

The theorem states that for a given configuration of nuclei, it is possible to calculate directly the force required to hold them; where it is understood that the nuclei are to be held fixed in position as point charges. Also, given any arbitrary number of parameters λ that specifies nuclear positions the expression of the force (in a generalized sense[15]) is

$$f_\lambda = -<\nabla_\lambda H> = -\int dv\Psi^*\nabla_\lambda H\Psi \tag{5}$$

where H is the (self-adjoint) Hamiltonian of the system, and Ψ are differentiable wave functions.

Let us here re-state the theorem in order to avoid its repetition in the text (see also [15]).

The wave function must be normalized at every λ, i.e.

$$(i)\int dv|\Psi|^2 = 1 \tag{6}$$

Steady state condition requires

$$(ii)H\Psi = E\Psi \tag{7}$$

where E, H and Ψ have to be thought depending on λ. The requirement that H is a self-adjoint operator means

$$(iii)\int dv\Psi^* H\nabla_\lambda\Psi = \int dv\nabla_\lambda\Psi H\Psi^* \tag{8}$$

and it is also valid the following relation

$$(iv)\frac{1}{i\hbar}[i\hbar\nabla_\lambda, H]\Psi = \nabla_\lambda H\Psi \tag{9}$$

The expectation value, is

$$E = \int dv\Psi^* H\Psi \tag{10}$$

that implies

$$\nabla_\lambda E = \int dv\Psi^*\nabla_\lambda H\Psi + \int dv\nabla_\lambda\Psi^* H\Psi + \int dv\Psi^* H\nabla_\lambda\Psi \tag{11}$$

From (i),(ii),(iii), and (iv) we obtain

$$\nabla_\lambda E = \int dv\Psi^*\nabla_\lambda H\Psi = \int dv\Psi^*\frac{1}{i\hbar}[i\hbar\nabla_\lambda, H]\Psi \tag{12}$$

We shall show in the next section, how to make use of the theorem (12) from another perspective.

GROUP VELOCITY

In this section it is shown how to calculate the group velocity of a quantal body.

We assume that the differentiable state Ψ of the system, varies parametrically with respect to a real vectorial field β.

We represent Ψ by complex differentiable functions, normalized in a suitable region D of space.

Also, we assume that the Hamiltonian $\hat{H}$ of the quantal body is *independent* of β and self-adjoint.

Let us define a generalized group velocity vector as:

$$\bar{V_\beta} = \hbar^{-1}\nabla_\beta E(\beta) \tag{13}$$

We consider here

$$\Psi_\beta = e^{i\bar{f}(\beta)\cdot\mathbf{r}}u_\beta \tag{14}$$

where $\bar{f}(\beta)$ is a real vectorial field function of β.
E is defined as follows

$$E(\beta) =< \Psi_\beta|\hat{H}|\Psi_\beta >=< u_\beta|\tilde{H}_\beta|u_\beta >= \int u_\beta^*\tilde{H}_\beta u_\beta dv \tag{15}$$

where dv is a volume element of space, and $\tilde{H}_\beta$ is obtained as

$$\tilde{H}_\beta = e^{-i\bar{f}(\beta)\cdot\mathbf{r}}\hat{H}e^{i\bar{f}(\beta)\cdot\mathbf{r}} \tag{16}$$

$\tilde{H}_\beta$ represents the Hamiltonian of the system[30] in the Hilbert space spanned by u_β, and it is parametrically dependent on β.

Inserting eq.(15) in eq.(13) we obtain,

$$\hbar\bar{V_\beta} = \nabla_\beta < \Psi_\beta|\hat{H}|\Psi_\beta > \; = \nabla_\beta < u_\beta|\tilde{H_\beta}|u_\beta > \tag{17}$$

We may consider $\bar{V_\beta}$ to be the averaged vector

$$\bar{V_\beta} = \frac{1}{\hbar} < u_\beta|\nabla_\beta\tilde{H_\beta}|u_\beta > \tag{18}$$

To prove that, under steady-state conditions, both definitions eq.(18) and eq(13), of group velocity become exactly equivalent, it is sufficient to make use of eq.(12), where we consider here λ being substituted by a Cartesian component of β. In the next section, as a matter of example, we show implications of eq.(18) in the theory of infinite periodic systems.

INFINITE PERIODIC SYSTEM

For an application of eq.(18), to an infinite periodic system, it is sufficient to make use of the $k-q$ representation, introduced by Zak[3].

Here $\mathbf{k}$ is the crystal momentum ([19]) and varies in the Brillouin zone of the reciprocal space while the quasi-coordinate $\mathbf{q}$ varies in the unit cell.

The $k-q$ representation of Schrödinger's equation, in the case of no external fields present in the system, is:

$$[\frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}})^2 + V(\mathbf{q})]C_{\mathbf{k}}(\mathbf{q}) = \epsilon C_{\mathbf{k}}(\mathbf{q}) \tag{19}$$

where

$$H_0 \equiv \frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}})^2 + V(\mathbf{q}) \tag{20}$$

as also stated in eq.(14) of reference [3], setting explicitly to zero the external fields.

Performing the following phase transformation

$$C_{\mathbf{k}}(\mathbf{q}) = e^{i\mathbf{k}\cdot\mathbf{q}}u_{\mathbf{k}}(\mathbf{q}) \tag{21}$$

the equation for $u_{\mathbf{k}}(\mathbf{q})$ becomes

$$[\frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k})^2 + V(\mathbf{q})]u_{\mathbf{k}}(\mathbf{q}) = \epsilon u_{\mathbf{k}}(\mathbf{q}) \tag{22}$$

where

$$H_{0,\mathbf{k}} \equiv \frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k})^2 + V(\mathbf{q}) \tag{23}$$

If we now consider a static external electromagnetic field (E_0, B^0) interacting with the QB, Schrödinger's equation in the $k-q$ representation becomes

$$\begin{aligned} H_{\mathbf{k}} =& [\frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k} + \frac{e}{c}B^0 \times i\nabla_{\mathbf{k}})^2 \\ &+ V(\mathbf{q}) + eE_0 \cdot i\nabla_{\mathbf{k}}]u_{\mathbf{k}}(\mathbf{q}) \\ &= \epsilon u_{\mathbf{k}}(\mathbf{q}) \end{aligned} \tag{24}$$

differently from the result shown by Zak, because of our choice of the vector potential.

In fact, in the $\mathbf{r}$ representation, we choose the vector potential as follows:

$$\mathbf{A}(\mathbf{r}) = B^0 \times \mathbf{r} \tag{25}$$

differently from the usual one used for the symmetric gauge [26].

It is clear that we can apply straightforwardly eq.(18), once we think of the region D as being the super-cell, and we substitute $\bar{f}(\beta) = \beta = \mathbf{k}$, and $\mathbf{r}$ with $\mathbf{q}$.

We can also evaluate eq.(24), at low energies, expanding brackets $(...)^2$ of eq.(24) in powers of $\frac{1}{c}$.

Taking only those terms proportional to $\frac{1}{c}$, we obtain

$$\begin{aligned} &[\frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k})^2 + \frac{e\mathbf{v}}{c} \cdot (B^0 \times i\nabla_{\mathbf{k}}) \\ &+ V(\mathbf{q}) + eE_0 \cdot i\nabla_{\mathbf{k}}]u_{\mathbf{k}}(\mathbf{q}) \\ &= \epsilon u_{\mathbf{k}}(\mathbf{q}) \end{aligned} \tag{26}$$

where $\mathbf{v} = \frac{1}{m}[-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k}]$, and the Hamiltonian of the problem is

$$\begin{aligned} \tilde{H}_{\mathbf{k}} \equiv& \frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k})^2 + \frac{e\mathbf{v}}{c} \cdot (B^0 \times i\nabla_{\mathbf{k}}) \\ &+ V(\mathbf{q}) + eE_0 \cdot i\nabla_{\mathbf{k}} = H_{0,\mathbf{k}} + \hat{\omega} \end{aligned} \tag{27}$$

The operator $\hat{\omega}$ is instead defined as

$$\hat{\omega} = eE_0 \cdot i\nabla_{\mathbf{k}} + \frac{e\mathbf{v}}{c} \cdot (B^0 \times i\nabla_{\mathbf{k}}) \tag{28}$$

Boundary conditions on the Bloch-like functions are the following

$$\begin{aligned} C_{\mathbf{k}+\mathbf{G_m}}(\mathbf{q}) &= C_{\mathbf{k}}(\mathbf{q}) \\ &\textit{and} \\ C_{\mathbf{k}}(\mathbf{q}+\mathbf{R_m}) &= e^{i\mathbf{k}\cdot\mathbf{R_m}} C_{\mathbf{k}}(\mathbf{q}) \end{aligned} \tag{29}$$

being $\mathbf{G_m}$ any reciprocal lattice vector and $\mathbf{R_m}$ any lattice vector[8, 19, 20].

Accordingly to (29), boundary conditions on functions $u_{\mathbf{k}}(\mathbf{q})$ are

$$\begin{aligned} u_{\mathbf{k}}(\mathbf{q}+\mathbf{R_m}) &= u_{\mathbf{k}}(\mathbf{q}) \\ &\textit{and} \\ u_{\mathbf{k}+\mathbf{G_m}}(\mathbf{q}) &= e^{-i\mathbf{G_m}\cdot\mathbf{q}} u_{\mathbf{k}}(\mathbf{q}) \end{aligned} \tag{30}$$

for every $\mathbf{G_m}$ and $\mathbf{R_m}$.

A particular solution then reads

$$C_{\mathbf{k}}(\mathbf{q}) = e^{i\mathbf{k}\cdot\mathbf{q}} u_{\mathbf{k}}(\mathbf{q}) \tag{31}$$

Making use of eq.(18) and eq.(24), the expression of the group velocity operator now becomes

$$\begin{aligned} \mathbf{V}^{(B^0)} &= \frac{1}{\hbar}\nabla_{\mathbf{k}} H_{\mathbf{k}} \\ &= \mathbf{v} + \frac{e}{mc} B^0 \times i\nabla_{\mathbf{k}} \end{aligned} \tag{32}$$

POWER

Here we show another possible application of eq.(32).

By eq.(32), we can calculate the group velocity of the system (in the case of $B^0 = 0$) as follows

$$\begin{aligned} \tilde{V}_{n\mathbf{k}} &= \frac{1}{\hbar} < u_{n\mathbf{k}} | \nabla_{\mathbf{k}} H_{\mathbf{k}} | u_{n\mathbf{k}} > \\ &= < u_{n\mathbf{k}} | \frac{1}{i\hbar}[i\nabla_{\mathbf{k}}, H_{\mathbf{k}}] | u_{n\mathbf{k}} > \end{aligned} \tag{33}$$

defining the density current vector as[19]

$$j_{n\mathbf{k}} = e\tilde{V}_{n\mathbf{k}} \tag{34}$$

We can then define the work, per unit time and per unit volume, made by the external electric field E_0 on the QB as

$$\begin{aligned} W = E_0 \cdot J &= E_0 \cdot \sum_n \int_{\Omega_{\mathbf{k_F}}} \frac{d\mathbf{k}}{(2\pi)^3} j_{n\mathbf{k}} \\ &= eE_0 \cdot \sum_n \int_{\Omega_{\mathbf{k_F}}} \frac{d\mathbf{k}}{(2\pi)^3} \tilde{V}_{n\mathbf{k}} \\ &= eE_0 \cdot \sum_n \int_{\Omega_{\mathbf{k_F}}} \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\hbar} \nabla_{\mathbf{k}} E_{n\mathbf{k}} \end{aligned} \tag{35}$$

where $\Omega_{\mathbf{k_F}}$ is the volume of $\mathbf{k}$ points such that their associated energies are smaller then the Fermi energy. A generalization of eq.(35) to the case $B^0 \neq 0$ will be given in the next section.

POWER IN A UNIFORM STATIC ELECTROMAGNETIC FIELD

By eq.(32), noting that the group velocity is not explicitly dependent on a uniform electrostatic field E_0 even being eventually present in the system, and bearing in mind eq.(34) and eq.(35), we can express the work per unit time and per unit volume done by the electromagnetic field on the body as

$$\begin{aligned} W = E_0 \cdot J = E^0 \cdot \int_V dV \mathbf{j}(\mathbf{k}) \\ = eE^0 \cdot \bar{\mathbf{v}} + \frac{4\pi e^2}{mc^2} \mathbf{S} \cdot \bar{\mathbf{d}} \end{aligned} \tag{36}$$

being $\mathbf{S} = \frac{\mathbf{c}}{\mathbf{4\pi}}(\mathbf{E_0} \times \mathbf{B^0})$ the Poynting vector[32] associated to the electromagnetic field, and

$$\mathbf{d} = \sum_n < u_{n,\mathbf{k}} | i\nabla_{\mathbf{k}} | u_{n,\mathbf{k}} > \tag{37}$$

$$\bar{\mathbf{P}} = e\bar{\mathbf{d}} = e \int_V \frac{dk}{(2\pi)^3} \mathbf{d} \tag{38}$$

where e is the electronic charge, and $\bar{\mathbf{P}}$ is the macroscopic polarization[7]. Eq.(37) and eq.(38) can be easily related to the dipole moment per unit volume of the system[7], that is expressed as a sum of Berry's connections[7]. A review of the physical and mathematical meaning of eq.(38) can be found in [6, 7, 8].

CONCLUSIONS

Within our model, concepts of group velocity and power density are directly related. Expression (36) may be useful for calculations of the measured power, adsorbed or released [22, 23, 24] by a quantal body in a transformation connecting two of its steady states; it may also be useful for calculations of Joule's effect, as the latter is directly related to the concept of power, and a quantification of the *heat* acquired or released by a QB, along a phase transformation between two of their steady states. Eq.(35), can be helpful for a more accurate theoretical description of materials that show an hysteresis loop[21],i.e during a phase transformation that changes their electrostatic potential in analogy with[7]. As a matter of example, we may think to apply our results to the study of dielectric properties of materials appertaining to the phenomenological *polar* class [21]).

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